

201-14864

Anh Nguyen

12/01/03 06:22 AM

To: NCIC HPV@EPA

CC:

Subject: HPV submission - CAS# 298-06-6

----- Forwarded by Anh Nguyen/DC/USEPA/US on 12/01/2003 06:20 AM -----

Cynthia Graham <cynthia.graham@bayerpolymers.com> on 11/26/2003 03:06:44 PM



To: "Oppt.ncic" <Oppt.ncic@epa.gov>, Chem.rtk/  
cc: Richard Hefter/DC/USEPA/US@EPA, Oscar Hernandez/DC/USEPA/US@EPA, Patrick Ragan  
<patrick.ragan@bayercropscience.com>, Greg Moerer <greg.moerer@bayercropscience.com>, Karen  
Hoffman/DC/USEPA/US@EPA

Subject: HPV submission - CAS# 298-06-6

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03 DEC -1 AM 9:17

Attached please find the

Cover letter (298066\_cvr ltr.pdf),  
Test plan (298066 test plan.pdf), and  
IUCLID document (298066\_IUCLID.pdf)

on O,O-diethyl dithiophosphate (CAS# 298-06-6) for submission to the US EPA  
HPV  
Challenge Program.

(See attached file: 298066\_IUCLID.pdf) (See attached file: 298066\_cvr  
ltr.pdf) (See attached file: 298066 test plan.pdf)

Best regards / Mit freundlichen Grüßen,

Cynthia Graham, Ph.D.

Bayer Polymers LLC

Product Safety & Regulatory Affairs

100 Bayer Road, Building #5

Pittsburgh, PA 15205-9741

Phone: 412-777-3933

Fax: 412-777-7484



Email: cynthia.graham@bayerpolymers.com 298066\_IUCLID.pdf 298066\_cvr ltr.pdf



298066 test plan.pdf

201-14864

**Bayer** 

November 26, 2003

Bayer Corporation  
100 Bayer Road  
Pittsburgh, PA 15205-9741  
Phone: 412 777-2000

Honorable Marianne Lamont Horinko  
Acting Administrator  
U.S. Environmental Protection Agency  
c/o P.O. Box 1473  
Merrifield, VA 22116

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03 DEC - 1 AM 9:17

Attn: Chemical Right-to-Know Program  
Re: HPV Registration No.

Dear Administrator Horinko;

Bayer CropScience LP is pleased to submit the proposed test plan along with the robust summaries in IUCLID format for O,O-diethyl dithiophosphate (CAS# 298-06-6). A separate letter is included to describe the process and transport of this substance to request "closed-system intermediate" status. The letter explaining intermediate status should remain confidential and should not be posted on the website.

Cynthia Graham, Ph.D. is our technical contact and can be reached at 412-777-3933 or by email at [cynthia.graham@bayerpolymers.com](mailto:cynthia.graham@bayerpolymers.com).

This submission is also being sent electronically to the following e-mail addresses:  
[Oppt.ncic@epa.gov](mailto:Oppt.ncic@epa.gov); [Chem.rtk@epa.gov](mailto:Chem.rtk@epa.gov).

Sincerely,

Janet M. Mostowy, Ph.D.  
Vice President  
Product Safety & Regulatory Affairs

Enclosures:

Test Plan; IUCLID data set on CAS# 56-93-9; Request for closed-system intermediate status

cc: Rich Hefter, EPA  
Karen Hoffman, EPA  
Oscar Hernandez, EPA  
Pat Ragan, Bayer CropScience  
Greg Moerer, Bayer CropScience

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**O,O-Diethyl dithiophosphate**

CAS # 298-06-6

**Test plan****Bayer CropScience LP**November 26, 2003

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RECEIVED  
OPPT CBIC  
03 DEC - 1 AM 9:18**Executive Summary**

Bayer CropScience LP (Bayer) hereby submits for review and public comment their test plan for O,O-diethyl dithiophosphate (CAS# 298-06-6) under the Environmental Protection Agency's High Production Volume (HPV) Chemical Challenge Program.

<u>IUPAC Name</u>	<u>Common Name</u>	<u>Abbreviation</u>	<u>CAS#</u>
O,O-diethyl dithiophosphate	diethyl acid	DEA	298-06-6

O,O-diethyl dithiophosphate is used as an intermediate in the production of an agricultural insecticide.

In consideration of animal welfare concerns to minimize the use of animals in the testing of chemicals, Bayer has conducted a thorough literature search for all available data, published and unpublished. Bayer has also performed an analysis of the adequacy of the existing data. Existing data indicates that this chemical is of high concern for aquatic toxicity, low concern as Persistent Organic Pollutants (POP), moderate concern for skin irritation, and low concern for acute mammalian toxicity. In a separate submission, Bayer has explained in detail that this substance is a closed-system intermediate and therefore a reduced data set is required. To fulfill the SIDS data set, an "*in vitro* Mammalian Cytogenetic Test" (OECD 473) and Teratogenicity study (OECD 414) on DEA is proposed for purposes of the HPV Program.

## **Closed System Intermediate Chemical Status**

A separate document is being submitted to EPA to describe the process, sites, and transport of DEA to explain “closed-system” intermediate status. This information is considered Confidential and therefore is not available to the public in this document.

## **Data Review**

### **Physicochemical properties:**

The properties of DEA can be found in various online databases and some endpoints were calculated with EPIWin Modeling Program. DEA is a liquid at ambient temperatures and decomposes before boiling. The calculated octanol/water partition coefficient is 1.17 and only the salt form is soluble in water. Data is available for all endpoints, no additional testing is proposed for purposes of the HPV Program (See Table 1 and IUCLID document).

### **Environmental Fate:**

Photodegradation was calculated as a half-life of 1.4 hours for DEA. Fugacity modeling demonstrates partitioning to the soil and water compartments. Biodegradation modeling demonstrates that DEA is biodegradable. In addition, a well documented study on various thiophosphates indicated complete mineralization within three weeks by acclimation. A water stability study demonstrated the nature of hydrolysis involves the attack of water molecule on the phosphorus of the di-ester involving P-O bond fission. Data is available for all endpoints, no additional testing is proposed for purposes of the HPV Program (See Table 1 and IUCLID document).

### **Ecotoxicology:**

Aquatic studies have been performed on *Salmo gairdineri*, *Poecilia reticulata* and on *Daphnia magna*. The 24 hour LC<sub>50</sub> of *Daphnia magna* = 0.54 mg/l (highly toxic). There are no studies on algae, however since DEA is highly toxic to *Daphnia*, additional testing on algae will not provide useful or relevant data for risk assessment. No additional testing is proposed for purposes of the HPV Program (See Table 1 and IUCLID document).

### **Mammalian Toxicology:**

Toxicity studies in animals show that DEA is of low acute toxicity by all routes of exposure: oral LD<sub>50</sub> 4510 mg/kg (rat); inhalation LC<sub>50</sub> 1640 mg/m<sup>3</sup> (rat); and dermal LD<sub>50</sub> > 2000 mg/kg (rabbit). (See Table 1 and IUCLID document).

There is an Ames study on DEA to fill the mutagenicity endpoint. No studies on chromosome aberration were located. An “*in vitro* Mammalian Cytogenetic Test” (OECD 473) on DEA is proposed for purposes of the HPV Program (See Table 1 and IUCLID document).

There were no repeat dose, fertility, nor developmental studies found. Since DEA is a closed system intermediate, the repeat dose and fertility studies are waived. A “Teratogenicity” study (OECD 414) on DEA is proposed for purposes of the HPV Program. (See Table 1 and IUCLID document).

### **“Beyond SIDS” Endpoints:**

Studies have been performed to investigate skin and eye irritation on DEA and found to be irritating to the skin and eyes of rabbits. (See Table 2 and IUCLID document).

### **Exposure:**

Since DEA is a closed-system intermediate, potential for exposure is minimal. Occupational exposure is controlled by good industrial hygiene practices and engineering controls. Environmental releases are controlled/prevented by engineering controls and careful monitoring. DEA is not present in the finished product, therefore there are no potential downstream exposures. DEA is not expected to pose a risk to human health or the environment during manufacture, formulation, and under normal conditions of anticipated use, if the recommended safe use and handling procedures are followed.

### **Conclusion**

Existing data indicates that this chemical is of high concern for aquatic toxicity, low concern as Persistent Organic Pollutants (POP), moderate concern for skin irritation, and low concern for acute mammalian toxicity. In a separate submission, Bayer has explained in detail that DEA is a closed-system intermediate and therefore a reduced data set is required. To fulfill the SIDS data set, an “*in vitro* Mammalian Cytogenetic Test” (OECD 473) and Teratogenicity study (OECD 414) on DEA is proposed for purposes of the HPV Program.

**Table 1. Available data for DEA**

Endpoint	DEA (CAS# 298-06-6)
<b>Physical-Chemical Data</b>	
Molecular weight	186.23
Physical state	liquid
Melting Point	Not applicable
Boiling Point	105-108 °C @ 20 hPa
Vapour Pressure	.077 hPa @ 25 °C
Partition Coefficient (logP <sub>ow</sub> )	1.17
Water Solubility	insoluble
<b>Environmental Fate</b>	
Photodegradation	T ½ = 1.4 hours
Fugacity (distribution)	Air – 1.06 % Water – 39.5% Soil – 59.3% Sediment – 0.152%
Biodegradability	Inherently biodegradable
Water Stability	See IUCLID document
<b>Ecotoxicology</b>	
Acute Fish Toxicity 96 hrs LC <sub>50</sub>	<i>Salmo gairdineri</i> 310-330 mg/l <i>Poecilia reticulata</i> 79 mg/l (24 hours)
Acute Invertebrate Toxicity 24 hrs LC <sub>50</sub>	<i>Daphnia magna</i> 0.54 mg/l
Algal Toxicity 96 hrs LC <sub>50</sub>	No data
<b>Mammalian Toxicology</b>	
Acute Toxicity	Oral LD <sub>50</sub> = 4510 mg/kg (rat) Inhalation LC <sub>50</sub> = 1640 mg/m3 (rat) Dermal LD <sub>50</sub> >2000 mg/kg (rabbit)
Mutagenicity	Ames (± activation) = negative
Chromosome Aberration	No data
Repeated Dose Toxicity	No data
Reproductive Toxicity	No data
Developmental Toxicity	No data

\* Robust summaries and References can be found in the IUCLID document.

**Table 2. “Beyond SIDS” data for DEA**

Endpoint	DEA (CAS# 298-06-6)
Skin Irritation	Slightly irritating (24 hrs, rabbit)
Eye Irritation	Highly irritating (24 hrs, rabbit)

\* Robust summaries and References can be found in the IUCLID document.

**Table 3. Test Plan for DEA**

Endpoint	Data Availability	Acceptable	Planned testing
<b>Physical-Chemical Data</b>			
Melting Point	✓	✓	
Boiling Point	✓	✓	
Vapour Pressure	✓	✓	
Partition Coefficient (logP <sub>ow</sub> )	✓	✓	
Water Solubility	✓	✓	
<b>Environmental Fate</b>			
Photodegradation	✓	✓	
Fugacity	✓	✓	
Biodegradability	✓	✓	
Water Stability	✓	✓	
<b>Ecotoxicology</b>			
Acute Fish Toxicity	✓	✓	
Acute Invertebrate Toxicity	✓	✓	
Algal Toxicity			Derogation statement
<b>Mammalian Toxicology</b>			
Acute Toxicity	✓	✓	
Mutagenicity	✓	✓	
Chromosome Aberration			OECD 473
Repeated Dose Toxicity	Not required 'Closed system intermediate'		
Reproductive Toxicity	Not required 'Closed system intermediate'		
Developmental Toxicity			OECD 414

✓ = data available and considered adequate.

201-14864B

# I U C L I D

## Data Set

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Existing Chemical : ID: 298-06-6  
CAS No. : 298-06-6  
EINECS Name : O,O-diethyl hydrogen phosphorodithioate  
EC No. : 206-055-9  
Molecular Formula : C4H11O2PS2

Producer related part  
Company : Bayer Corporation  
Creation date : 08.11.2002

Substance related part  
Company : Bayer Corporation  
Creation date : 08.11.2002

Status :  
Memo : Bayer CropScience LP - US EPA HPV submission

Printing date : 26.11.2003  
Revision date :  
Date of last update : 26.11.2003

Number of pages : 25

Chapter (profile) : Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10  
Reliability (profile) : Reliability: without reliability, 1, 2, 3, 4  
Flags (profile) : Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE),  
Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

# 1. General Information

**Id** 298-06-6

**Date** 26.11.2003

## 1.0.1 APPLICANT AND COMPANY INFORMATION

**Type** : importer of product  
**Name** : Bayer Corporation  
**Contact person** :  
**Date** :  
**Street** : 100 Bayer Road, Building #5  
**Town** : PA 15205-9741 Pittsburgh  
**Country** : United States  
**Phone** :  
**Telefax** :  
**Telex** :  
**Cedex** :  
**Email** :  
**Homepage** :

13.11.2003

## 1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

## 1.0.3 IDENTITY OF RECIPIENTS

## 1.0.4 DETAILS ON CATEGORY/TEMPLATE

### 1.1.0 SUBSTANCE IDENTIFICATION

**IUPAC Name** : Phosphorodithioic acid, O,O-diethyl ester  
**Smiles Code** : O(P(OCC)(S)=S)CC  
**Molecular formula** : C4 H11 O2 P1 S2  
**Molecular weight** : 186.23  
**Petrol class** :

08.10.2003

### 1.1.1 GENERAL SUBSTANCE INFORMATION

**Purity type** : typical for marketed substance  
**Substance type** : organic  
**Physical status** : liquid  
**Purity** :  
**Colour** : colorless to blue-green  
**Odour** :

**Source** : Merck KGaA, Frankfurter Str. 250, D-64293 Darmstadt, Germany.  
www.chemdata.de/  
Sigma-Aldrich, 3050 Spruce Street, St. Louis Missouri 63103, USA

11.11.2003

### 1.1.2 SPECTRA

## 1. General Information

**Id** 298-06-6  
**Date** 26.11.2003

### 1.2 SYNONYMS AND TRADENAMES

Dithiophosphoric acid O,O-diethyl ester

11.11.2003

13.11.2003

### 1.3 IMPURITIES

### 1.4 ADDITIVES

### 1.5 TOTAL QUANTITY

### 1.6.1 LABELLING

### 1.6.2 CLASSIFICATION

### 1.6.3 PACKAGING

### 1.7 USE PATTERN

### 1.7.1 DETAILED USE PATTERN

### 1.7.2 METHODS OF MANUFACTURE

### 1.8 REGULATORY MEASURES

### 1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

### 1.8.2 ACCEPTABLE RESIDUES LEVELS

### 1.8.3 WATER POLLUTION

### 1.8.4 MAJOR ACCIDENT HAZARDS

## 1. General Information

**Id** 298-06-6  
**Date** 26.11.2003

### 1.8.5 AIR POLLUTION

### 1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

### 1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

### 1.9.2 COMPONENTS

### 1.10 SOURCE OF EXPOSURE

### 1.11 ADDITIONAL REMARKS

### 1.12 LAST LITERATURE SEARCH

**Type of search** : Internal and External  
**Chapters covered** : 3, 4, 5  
**Date of search** : 01.07.2003

26.11.2003

### 1.13 REVIEWS

## 2. Physico-Chemical Data

Id 298-06-6  
Date 26.11.2003

### 2.1 MELTING POINT

Method : other  
Year :  
GLP : no  
Test substance : as prescribed by 1.1 - 1.4  
  
Remark : Not applicable; substance is a liquid at ambient temperature  
Flag : Critical study for SIDS endpoint  
11.11.2003

### 2.2 BOILING POINT

Value : 105 - 108 °C at 20 hPa  
Decomposition :  
Method : other: no data  
Year :  
GLP : no data  
Test substance : as prescribed by 1.1 - 1.4  
  
Flag : Critical study for SIDS endpoint  
11.11.2003 (1)  
  
Decomposition : yes  
Method : other: no data  
Year :  
GLP : no data  
Test substance : as prescribed by 1.1 - 1.4  
  
Remark : Decomposition at temperatures > 150 degree C  
11.11.2003 (1)

### 2.3 DENSITY

Type : density  
Value : 1.17 g/cm3 at 20 °C  
Method : other: no data  
Year :  
GLP : no data  
Test substance : as prescribed by 1.1 - 1.4  
  
Flag : Critical study for SIDS endpoint  
11.11.2003 (1)  
  
Type : relative density  
Value : 1.111  
Method : other: no data  
Year :  
GLP : no data  
Test substance : as prescribed by 1.1 - 1.4  
  
11.11.2003 (2)

## 2. Physico-Chemical Data

Id 298-06-6

Date 26.11.2003

### 2.3.1 GRANULOMETRY

### 2.4 VAPOUR PRESSURE

**Value** : .077 hPa at °C  
**Decomposition** :  
**Method** : other (calculated): MPBPWIN (v1.41)  
**Year** :  
**GLP** : no  
**Test substance** : other TS: molecular structure

**Result** : Vapor Pressure Estimations (25 deg C):  
(Using BP: 235.63 deg C (estimated))  
(MP not used for liquids)  
VP: 0.0611 mm Hg (Antoine Method)  
VP: 0.0554 mm Hg (Modified Grain Method)  
VP: 0.0957 mm Hg (Mackay Method)  
Selected VP: 0.0583 mm Hg (Mean of Antoine & Grain methods)

**Reliability** : (2) valid with restrictions  
Accepted calculation method

**Flag** : Critical study for SIDS endpoint  
08.10.2003 (3)

### 2.5 PARTITION COEFFICIENT

**Partition coefficient** :  
**Log pow** : 1.17 at 25°C  
**Method** : other (calculated)  
**Year** :  
**GLP** : no  
**Test substance** : other TS: molecular structure

**Reliability** : (2) valid with restrictions  
Accepted calculation method

**Flag** : Critical study for SIDS endpoint  
28.10.2003 (4)

**Partition coefficient** :  
**Log pow** : at 23 °C  
**Method** : other (measured)  
**Year** :  
**GLP** : no  
**Test substance** : other TS: diethylphosphorodithioic acid; purity not noted

**Method** : The solvent distribution of diethylphosphorodithioic acid was investigated at room temperature (22-23 degree C) by using 100 ml separation funnels: 10 ml of aqueous solution of 1 M ionic strength were shaken with 10 ml of organic solvent (butanol or benzene) containing known amounts of test substance. After 20 minutes the phases were separated. The concentration of test substance was determined by iodometric titration or potentiation titration with AgNO<sub>3</sub>. The volume changes caused by reciprocal solubility in the water-benzene can be neglected. For the water-butanol system, volume corrections were made.

**Result** :  

	pH50	logP	pKa
water/benzene system:	0.30	0.37	-0.07
water/n-butanol system:	0.70	0.55	0.15

  
28.10.2003 (5)

## 2. Physico-Chemical Data

Id 298-06-6

Date 26.11.2003

Partition coefficient : octanol-water  
Log pow : 2.24 at 25 °C  
Method : other (calculated): KOWWIN Program (v1.65)  
Year :  
GLP : no  
Test substance : other TS: molecular structure

Result : SMILES : O(P(OCC)(S)=S)CC  
CHEM : Phosphorodithioic acid, O,O-diethyl ester  
MOL FOR: C4 H11 O2 P1 S2  
MOL WT : 186.23

-----+-----+-----+-----+-----					
TYPE	NUM	LOGKOW	FRAGMENT DESCRIPTION	COEFF	VALUE
-----+-----+-----+-----+-----					
Frag	2	-CH3	[aliphatic carbon]	0.5473	1.0946
Frag	2	-CH2-	[aliphatic carbon]	0.4911	0.9822
Frag	1	S=P	[thio=phosphorus]	-0.6587	-0.6587
Frag	2	-O-P	[aliphatic attach]	-0.0162	-0.0324
Frag	1	-S-P	[sulfur, phosphorus attach]	0.6270	0.6270
Const			Equation Constant		0.2290
-----+-----+-----+-----+-----					

Log Kow = 2.2417

Reliability : (2) valid with restrictions  
Accepted calculation method

28.10.2003

(3)

### 2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in : Water  
Description : not soluble  
Stable :  
Deg. product :  
Method : other: no data  
Year :  
GLP : no data  
Test substance : as prescribed by 1.1 - 1.4

11.11.2003

(1)

### 2.6.2 SURFACE TENSION

### 2.7 FLASH POINT

### 2.8 AUTO FLAMMABILITY

### 2.9 FLAMMABILITY

### 2.10 EXPLOSIVE PROPERTIES

## 2.11 OXIDIZING PROPERTIES

## 2.12 DISSOCIATION CONSTANT

**Method** : other  
**Year** :  
**GLP** : no  
**Test substance** : other TS: diethylphosphorodithioic acid; purity not noted

**Method** : The solvent distribution of diethylphosphorodithioic acid was investigated at room temperature (22-23 degree C) by using 100 ml separation funnels: 10 ml of aqueous solution of 1 M ionic strength were shaken with 10 ml of organic solvent (butanol or benzene) containing known amounts of test substance. After 20 minutes the phases were separated.  
The concentration of test substance was determined by iodometric titration or potentiation titration with AgNO<sub>3</sub>. The volume changes caused by reciprocal solubility in the water-benzene can be neglected. For the water-butanol system, volume corrections were made.

<b>Result</b>	:	<u>pH50</u>	<u>logP</u>	<u>pKa</u>
		water/benzene system:	0.30	0.37 -0.07
		water/n-butanol system:	0.70	0.55 0.15

28.10.2003

(5)

## 2.13 VISCOSITY

## 2.14 ADDITIONAL REMARKS

### 3. Environmental Fate and Pathways

Id 298-06-6

Date 26.11.2003

#### 3.1.1 PHOTODEGRADATION

**Type** : air  
**INDIRECT PHOTOLYSIS**  
**Sensitizer** : OH  
**Conc. of sensitizer** : 1500000 molecule/cm<sup>3</sup>  
**Rate constant** : .00000000000916 cm<sup>3</sup>/(molecule\*sec)  
**Degradation** : 50 % after 1.4 hour(s)  
**Deg. product** :  
**Method** : other (calculated): AOP Program (v1.91)  
**Year** :  
**GLP** : no  
**Test substance** : other TS: molecular structure

**Remark** : The U.S. EPA uses a 12-hr day because OH radicals exist only during sunlight hours...the 12-hr period is an average daylight time for a whole year. The U.S. EPA uses an OH concentration of 1.5E6 which is an average concentration for daylight hours only

**Reliability** : (2) valid with restrictions  
Accepted calculation method

**Flag** : Critical study for SIDS endpoint  
08.10.2003 (3)

#### 3.1.2 STABILITY IN WATER

**Type** : abiotic  
**GLP** : no data  
**Test substance** : other TS: diethyl dithiophosphate; BDH quality

**Method** : "Allen's" modified method of colorimetry, in aqueous solutions from 0.1 to 7.0 mol/dm<sup>3</sup> HCL at 98 degree C.

**Remark** : Diethyl dithiophosphate in acid media occurs as both conjugate acid species and neutral species. Comparative data support the bimolecular nature of hydrolysis involving attack of water molecule on phosphorus of the diester involving P-O bond fission.

**Result** : Experimental and Estimated data for the hydrolysis of diethyl dithiophosphate at 98 degree C

HCL (mol/dm <sup>3</sup> )	Ke x 10e4 (min-1) (experimental)	Ke x 10e4 (min-1) (estimated)
0.1	11.32	12.68
0.2	12.74	12.87
0.5	13.02	13.45
1.0	13.75	14.44
2.0	16.86	16.58
3.0	18.14	18.91
4.0	22.22	21.45
5.0	16.44	16.51
6.0	15.16	14.60
7.0	13.75	13.22

**Reliability** : (2) valid with restrictions  
Meets generally accepted scientific standards, well documented and acceptable for assessment.

**Flag** : Critical study for SIDS endpoint  
28.10.2003 (6)

### 3. Environmental Fate and Pathways

Id 298-06-6

Date 26.11.2003

#### 3.1.3 STABILITY IN SOIL

#### 3.2.1 MONITORING DATA

#### 3.2.2 FIELD STUDIES

#### 3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type : fugacity model level III  
Method : other: EPIWIN modelling program  
Year :

Remark : Modeling was performed using equal releases (1,000 kg/hr) and equal distribution to all compartments.

Result : Level III Fugacity Model (Full-Output):

=====

Chem Name : Phosphorodithioic acid, O,O-diethyl ester  
Molecular Wt: 186.23  
Henry's LC : 0.000371 atm-m<sup>3</sup>/mole (Henrywin program)  
Vapor Press : 0.0583 mm Hg (Mppbpwin program)  
Log Kow : 2.24 (Kowwin program)  
Soil Koc : 71.2 (calc by model)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	1.06	2.8	1000
Water	39.5	360	1000
Soil	59.3	360	1000
Sediment	0.152	1.44e+003	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	8.3e-012	1.57e+003	63.3	52.2	2.11
Water	2.35e-009	454	236	15.1	7.86
Soil	1.95e-008	681	0	22.7	0
Sediment	1.67e-009	0.437	0.0182	0.0146	0.000605

Persistence Time: 199 hr  
Reaction Time: 221 hr  
Advection Time: 2e+003 hr  
Percent Reacted: 90  
Percent Advected: 9.97

Reliability : (2) valid with restrictions  
Accepted calculation method

Flag : Critical study for SIDS endpoint

11.11.2003

(3)

#### 3.3.2 DISTRIBUTION

#### 3.4 MODE OF DEGRADATION IN ACTUAL USE

### 3. Environmental Fate and Pathways

Id 298-06-6

Date 26.11.2003

#### 3.5 BIODEGRADATION

Type : aerobic  
Result : inherently biodegradable  
Deg. product :  
Method : other: BIOWIN (v4.01)  
Year :  
GLP : no  
Test substance : other TS: molecular structure

Result : ----- BIOWIN v4.01 Results-----

Linear Model Prediction : Biodegrades Fast  
Non-Linear Model Prediction: Biodegrades Fast  
Ultimate Biodegradation Timeframe: Weeks  
Primary Biodegradation Timeframe: Days-Weeks  
MITI Linear Model Prediction : Does Not Biodegrade Fast  
MITI Non-Linear Model Prediction: Does Not Biodegrade Fast

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
MolWt  *		Molecular Weight Parameter		-0.0887
Const  *		Equation Constant		0.7475
=====				
RESULT		LINEAR BIODEGRADATION PROBABILITY		0.6589
=====				
TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
MolWt  *		Molecular Weight Parameter		-2.6444
Const  *		Equation Constant		0.5901
=====				
RESULT		NON-LINEAR BIODEGRADATION PROBABILITY		0.5901
=====				

A Probability Greater Than or Equal to 0.5 indicates --> **Biodegrades Fast**

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
MolWt  *		Molecular Weight Parameter		-0.4115
Const  *		Equation Constant		3.1992
=====				
RESULT		SURVEY MODEL - ULTIMATE BIODEGRADATION		2.7876
=====				

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
MolWt  *		Molecular Weight Parameter		-0.2687
Const  *		Equation Constant		3.8477
=====				
RESULT		SURVEY MODEL - PRIMARY BIODEGRADATION		3.5791
=====				

**Result Classification:** 5.00 -> hours **4.00 -> days** **3.00 -> weeks**  
2.00 -> months 1.00 -> longer (Primary & Ultimate)

Reliability : (2) valid with restrictions  
Accepted calculation method

28.10.2003

(3)

Type : aerobic  
Inoculum : activated sludge, adapted

### 3. Environmental Fate and Pathways

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<b>Concentration</b>	: 500 mg/l related to Test substance related to
<b>GLP</b>	: no data
<b>Test substance</b>	: other TS: O,O-dimethyl ammonium phosphorodithioate [DMDTP] (purchased from Aldrich Chemical Co. Milwaukee, USA) and O,O-diethyl ammonium phosphorodithioate (purchased from Strem Chemicals, Danvers, USA)
<b>Method</b>	: The sludge was activated by a fill-and-draw method in a batch system. The activated sludge was washed 3 times with tap water and suspended in tap water to a mixed liquor suspended solid concentration of 5000 mg/l. To 1.5 liter of mixed liquor was added 500 mg/l of test substance and cultured with aeration at 30 degree C. The pH of the mixture was maintained at 7.0. At intervals, 15 ml portions were removed and filtered for analysis. DMDTP was measured colorimetrically at 420 nm. Water-soluble TOC was estimated with a Beckmanm model 102A TOC analyzer. Inorganic orthophosphate was estimated by the colorimetric method of molybdenum blue with the use of stannous chloride as a reducing agent. The degradation products in the extracellular solution were separated with thin-layer chromatography.
<b>Remark</b>	: The degradation pathway of DMDTP by activated sludge is DMDTP -> DMTP -> DMP -> MP -> P.
<b>Result</b>	: A drop in pH was observed in mixed liquor during acclimation and the pH adjusted to 7.0 whenever the medium was replaced. The activated sludge did not degrade DMDTP to inorganic phosphate for three months. When the acclimation was carried out using a pH controller to maintain the pH at 7.0, the DMDTP disappeared after 6 days.  This adapted sludge was able to degrade 500 mg/l of DMDTP in 1 day when the pH range was 5.0 to 7.5. Degradation did not occur at pH lower than 4.5 or higher than 8.5.
<b>Conclusion</b>	: Activated sludge degraded all test substances to inorganic phosphate by acclimation within 3 weeks.
<b>Reliability</b>	: (2) valid with restrictions
<b>Flag</b>	: Critical study for SIDS endpoint
11.11.2003	(7)

#### 3.6 BOD5, COD OR BOD5/COD RATIO

#### 3.7 BIOACCUMULATION

<b>Species</b>	: other
<b>Exposure period</b>	: at 25 °C
<b>Concentration</b>	:
<b>BCF</b>	: 10.62
<b>Elimination</b>	:
<b>Method</b>	: other: (calculated) BCF Program (v2.15)
<b>Year</b>	:
<b>GLP</b>	: no
<b>Test substance</b>	: other TS: molecular structure
<b>Result</b>	: ----- Bcfwin v2.15 ----- Log Kow (estimated) : 2.24 Log Kow (experimental): not available from database Log Kow used by BCF estimates: 2.24  Equation Used to Make BCF estimate: Log BCF = 0.77 log Kow - 0.70 + Correction

### 3. Environmental Fate and Pathways

**Id** 298-06-6  
**Date** 26.11.2003

Correction(s): No Applicable Correction Factors

13.11.2003 Estimated Log BCF = 1.026 (BCF = 10.62) (3)

#### 3.8 ADDITIONAL REMARKS

## 4.1 ACUTE/PROLONGED TOXICITY TO FISH

<b>Type</b>	:	static
<b>Species</b>	:	Salmo gairdneri (Fish, estuary, fresh water)
<b>Exposure period</b>	:	96 hour(s)
<b>Unit</b>	:	mg/l
<b>LC50</b>	:	310 - 330
<b>Limit test</b>	:	
<b>Analytical monitoring</b>	:	no data
<b>Method</b>	:	
<b>Year</b>	:	
<b>GLP</b>	:	no
<b>Test substance</b>	:	other TS: Phosphorodithioic acid, O,O-diethyl ester, sodium salt - Sodium Aerofloat (commercial product)
<b>Method</b>	:	Fingerlings from three different egg sources were used. The fingerlings, ranged in weight 1-10 g were allowed to acclimate for 24 hours. 20 fish were added to each test aquaria. Approximately one hour after the fish were transferred, the sample (previously dissolved in an aliquot of experimental water) was added. Water temperature was maintained at 12 (+/-1) degree C. Median lethal concentrations were determined by plotting median survival times, LC50, as a function of the logarithm of the concentration.
<b>Result</b>	:	LC50 = 400 - 410 ppm at 12 degrees C LC50 = 310 - 330 ppm at 16 degrees C
<b>Test condition</b>	:	The experimental water used was naturally hard spring water used in a trout fish hatchery. The volume of water was adjusted to maintain a ratio of 2g wet fish per liter of water. pH = 8.6; total hardness = 348 ppm; carbonate hardness = 203 ppm; oxygen saturation was maintained by bubbling air into the water.
<b>Reliability</b>	:	(2) valid with restrictions Meets generally accepted scientific standards, well documented and acceptable for assessment.
<b>Flag</b>	:	Critical study for SIDS endpoint
26.11.2003		(8)
<b>Type</b>	:	
<b>Species</b>	:	Poecilia reticulata (Fish, fresh water)
<b>Exposure period</b>	:	24 hour(s)
<b>Unit</b>	:	mg/l
<b>LC50</b>	:	79
<b>Method</b>	:	other: no data
<b>Year</b>	:	
<b>GLP</b>	:	no data
<b>Test substance</b>	:	as prescribed by 1.1 - 1.4
<b>Reliability</b>	:	(2) valid with restrictions Data from Handbook or collection of data
<b>Flag</b>	:	Critical study for SIDS endpoint
26.11.2003		(1)
<b>Type</b>	:	other: SAR
<b>Species</b>	:	
<b>Exposure period</b>	:	96 hour(s)
<b>Unit</b>	:	mg/l
<b>LC50</b>	:	10.982
<b>Method</b>	:	other: ECOSAR Program (v0.99g)
<b>Year</b>	:	
<b>GLP</b>	:	no

## 4. Ecotoxicity

Id 298-06-6

Date 26.11.2003

**Test substance** : other TS: molecular structure

**Remark** : ECOSAR Class: Esters (phosphate)

**Reliability** : (2) valid with restrictions  
Accepted calculation method

26.11.2003

(3)

### 4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

**Type** :

**Species** : Daphnia magna (Crustacea)

**Exposure period** : 24 hour(s)

**Unit** : mg/l

**EC50** : .54

**Analytical monitoring** : no data

**Method** : OECD Guide-line 202

**Year** :

**GLP** : no data

**Test substance** : other TS: diethyldithiophosphate; purity = 90%; obtained from Aldrich, Germany

**Reliability** : (2) valid with restrictions  
Guideline study

**Flag** : Critical study for SIDS endpoint

07.10.2003

(9)

### 4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

### 4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

**Type** : aquatic

**Species** : Photobacterium phosphoreum (Bacteria)

**Exposure period** : 30 minute(s)

**Unit** : mg/l

**EC10** : 3.13 -

**Analytical monitoring** : no data

**Method** : other: Microtox assay

**Year** :

**GLP** : no data

**Test substance** : other TS: diethyldithiophosphate; purity = 90%; obtained from Aldrich, Germany

**Test condition** : The inhibition of bioluminescence was measured according to Beckman Microtox system operating manual (1982) in a saline solution (2% NaCl in water) at a temperature of 15 degrees C, after a 30 minute incubation.

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(9)

### 4.5.1 CHRONIC TOXICITY TO FISH

### 4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

## 4. Ecotoxicity

**Id** 298-06-6  
**Date** 26.11.2003

**4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS**

**4.6.2 TOXICITY TO TERRESTRIAL PLANTS**

**4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS**

**4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES**

**4.7 BIOLOGICAL EFFECTS MONITORING**

**4.8 BIOTRANSFORMATION AND KINETICS**

**4.9 ADDITIONAL REMARKS**

## 5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

## 5.1.1 ACUTE ORAL TOXICITY

Type : LD50  
Value : 4510 mg/kg bw  
Species : rat  
Strain :  
Sex :  
Number of animals :  
Vehicle :  
Doses :  
Method :  
Year :  
GLP :  
Test substance : other TS: Phosphorodithioic acid, O,O-diethyl ester; purity not noted  
  
Reliability : (2) valid with restrictions  
Data from Handbook or collection of data  
Flag : Critical study for SIDS endpoint  
13.11.2003 (10)

## 5.1.2 ACUTE INHALATION TOXICITY

Type : LC50  
Value : 1640 mg/m3  
Species : rat  
Strain :  
Sex :  
Number of animals :  
Vehicle :  
Doses :  
Exposure time : 4 hour(s)  
Method : other: no data  
Year :  
GLP : no data  
Test substance : other TS: Phosphorodithioic acid, O,O-diethyl ester; purity not noted  
  
Remark : TOXIC EFFECTS:  
Behavioral - Somnolence (general depressed activity)  
Lung, Thorax, or Respiration - Dyspnea  
Nutritional and Gross Metabolic - Weight loss or decreased weight gain  
  
Reliability : (2) valid with restrictions  
Data from Handbook or collection of data  
Flag : Critical study for SIDS endpoint  
13.11.2003 (11)

## 5.1.3 ACUTE DERMAL TOXICITY

Type : LD50  
Value : > 2000 mg/kg bw  
Species : rabbit  
Strain : New Zealand white  
Sex : male/female

## 5. Toxicity

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Date 26.11.2003

Number of animals : 4  
Vehicle : water  
Doses : 2000 mg/kg bw  
Method : OECD Guide-line 402 "Acute dermal Toxicity"  
Year :  
GLP : no  
Test substance : other TS: sodium O,O-diethyl phosphorodithionate (CAS# 3338-24-7); commercial product; purity not indicated

Result : 

Sex	Dose	# Deaths/# Symptoms/# exposed
Male	2000 mg/kg	0/0/2
Female	2000 mg/kg	0/0/2

Reliability : (2) valid with restrictions  
Guideline study with acceptable restrictions;  
only 2 animals/sex were used in a limit test

Flag : Critical study for SIDS endpoint

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(12)

### 5.1.4 ACUTE TOXICITY, OTHER ROUTES

#### 5.2.1 SKIN IRRITATION

Species : rabbit  
Concentration : 500 mg  
Exposure : Occlusive  
Exposure time : 24 hour(s)  
Number of animals :  
Vehicle :  
PDII :  
Result : slightly irritating  
Classification :  
Method : Draize Test  
Year :  
GLP : no data  
Test substance : other TS: Phosphorodithioic acid, O,O-diethyl ester; purity not noted

Reliability : (2) valid with restrictions  
Data from Handbook or collection of data

13.11.2003

(10)

#### 5.2.2 EYE IRRITATION

Species : rabbit  
Concentration : .1 mg  
Dose :  
Exposure time : 24 hour(s)  
Comment :  
Number of animals :  
Vehicle :  
Result : highly irritating  
Classification :  
Method :  
Year :  
GLP : no data  
Test substance : other TS: Phosphorodithioic acid, O,O-diethyl ester; purity not noted

Reliability : (2) valid with restrictions

13.11.2003

Data from Handbook or collection of data

(10)

**5.3 SENSITIZATION****5.4 REPEATED DOSE TOXICITY****5.5 GENETIC TOXICITY 'IN VITRO'**

**Type** : Ames test  
**System of testing** : Salmonella typhimurium TA1538, TA98, TA1535, TA100, TA1537  
**Test concentration** :  
**Cycotoxic concentr.** :  
**Metabolic activation** : with and without  
**Result** : negative  
**Method** : OECD Guide-line 471  
**Year** :  
**GLP** : no data  
**Test substance** : other TS: O,O-diethyldithiophosphate; purity not noted  
  
**Remark** : Bacterial strains were received from Professor B.N. Ames, University of California, US.  
**Reliability** : (2) valid with restrictions  
Meets generally accepted scientific standards  
**Flag** : Critical study for SIDS endpoint  
13.11.2003

(13)

**5.6 GENETIC TOXICITY 'IN VIVO'****5.7 CARCINOGENICITY****5.8.1 TOXICITY TO FERTILITY****5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY****5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES**

**Type** : other: inhibition of acetylcholinesterase  
**In vitro/in vivo** : In vitro  
**Result** : > 1000 mg/l of dithiophosphate was needed for complete inhibition of AChE  
  
**Method** :  
**Year** :  
**GLP** : no data  
**Test substance** : other TS: diethyldithiophosphate; purity = 90%; obtained from Aldrich, Germany

**Method**

: To 1.0 ml of enzyme solution (containing 15 ug horse blood serum in 70 mM phosphate buffer pH 6.5) 1.0 ml of varying aqueous dilutions of insecticide solution was added, mixed, and incubated for 5 minutes at 20 degree C. After addition of 0.5 ml substrate solution (containing 4.0 mg butyrylthiocholin iodide in 70 mM phosphate buffer pH 6.5) the mixture was incubated for 5 minutes at 37 degree C in a water bath. Then 1.0 ml staining solution (containing 0.1 mg dichlorophenolindophenol in 70 mM phosphate buffer pH 6.5) was added and incubated at 37 degree C. After 5 minutes, the color was assessed visually - a dark blue color indicates total inhibition of AChE.

07.10.2003

(9)

**5.9 SPECIFIC INVESTIGATIONS****5.10 EXPOSURE EXPERIENCE****5.11 ADDITIONAL REMARKS**

### 6.1 ANALYTICAL METHODS

### 6.2 DETECTION AND IDENTIFICATION

## **7. Eff. Against Target Org. and Intended Uses**

**Id** 298-06-6  
**Date** 26.11.2003

**7.1 FUNCTION**

**7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED**

**7.3 ORGANISMS TO BE PROTECTED**

**7.4 USER**

**7.5 RESISTANCE**

**8.1 METHODS HANDLING AND STORING**

**8.2 FIRE GUIDANCE**

**8.3 EMERGENCY MEASURES**

**8.4 POSSIB. OF RENDERING SUBST. HARMLESS**

**8.5 WASTE MANAGEMENT**

**8.6 SIDE-EFFECTS DETECTION**

**8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER**

**8.8 REACTIVITY TOWARDS CONTAINER MATERIAL**

- (1) Merck KGaA, Frankfurter Str. 250, D-64293 Darmstadt, Germany. [www.chemdata.de/](http://www.chemdata.de/)
- (2) Sigma-Aldrich, 3050 Spruce Street, St. Louis Missouri 63103, USA
- (3) EPIWin Modeling Program. (version 3.11) 2000. Developed by the EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC). copyright 2000 U.S. Environmental Protection Agency
- (4) Advanced Chemistry Development (ACD) Software Solaris v.4.67 (copyright 1994-2002 ACD)
- (5) Curtui M, Marcu G, and Haiduc I. 1976. Solvent Extraction of Uranium (VI) with dialkylphosphorodithioic acids (III). *Studia Univ. Babes-Bolyai Chemia*. 21:74-79
- (6) Patil R, Shinde CP, Samadhia A. 1997. Kinetics and mechanism of hydrolysis of diethyl dithiophosphate in Acid Media. *Asian J. Chemistry*. 9(3):407-410.
- (7) Kanagawa T, Dazai M, Takahara Y. 1980. Degradation of O,O-Dimethyl Phosphorodithioate by Activated Sludge. *Agric. Biol. Chem.* 44(11):2631-2635.
- (8) Fuerstenau MC, Wakawa BM, et al. 1974. Toxicity of selected sulfhydryl collectors to rainbow trout. *Transactions. Society of Mining Engineers*. 256(4): 337-341.
- (9) Galli R, Rich H W, Scoltz R. 1994. Toxicity of organophosphate insecticides and their metabolites to the water flea, *Daphnia magna*, the Microtox test and an acetylcholinesterase inhibition test. *Aquatic Tox.* 30:259-269.
- (10) Marhold, J. 1986. "Prehled Prumyslove Toxicologie; Organicke Latky." Prague, Czechoslovakia, Avicemun. as reported in "Registry of Toxic Effects of Chemical Substances" compiled by the National Institute for Occupational Safety and Health of the U.S. Department of Health and Human Services. 1993-2003.
- (11) National Technical Information Service. (Springfield, VA 22161) Formerly U.S. Clearinghouse for Scientific & Technical Information. as reported in the "Registry of Toxic Effects of Chemical Substances" compiled by the National Institute for Occupational Safety and Health of the U.S. Department of Health and Human Services. 1993-2003.
- (12) Mobay Chemical Corporation. 1972. CHEMAGRO Agricultural Division Study Report No. 35287
- (13) Szarapinska-Kwaszewska, J. and Rozalska, M. 1982. Study of environmental carcinogens. I. Mutagenic activity of organophosphate pesticides. *Inst. Patol., Akad. Med., Lodz, Poland. Bromatol. Chem. Toksykol.* 15(1-2):89-93

## 10. Summary and Evaluation

**Id** 298-06-6  
**Date** 26.11.2003

### 10.1 END POINT SUMMARY

### 10.2 HAZARD SUMMARY

### 10.3 RISK ASSESSMENT